

Antiferromagnetic Order in a Spin-Orbit Coupled Bose-Einstein Condensate

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Spin-orbit coupling related new physics and quantum magnetism are two branches of great interest both in condensed matter physics and in cold atomic physics. With the introduction of a Rashba-like SOC into a Bose-Einstein condensate (BEC) loaded in a two-dimensional bipartite optical square lattice, we find that the ground state of the BEC always favors a coherent condensate than a fragmented condensate and always exhibits very large degeneracy, and most importantly, an antiferromagnetic order of quantum nature emerges when parameters satisfy certain condition. This provides an ideal platform to study the interplay of antiferromagnetic phase and superfluid phase.

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Introduction.— Due to the great impact of spin-orbit coupling (SOC) on the band structure of both fermionic systems and bosonic systems, the study of new physics related to SOC has been being of central interest both in condensed matter community and in cold atomic community for many years [1–8]. For fermionic systems with certain symmetries, it is found that in the appearance of SOC, the energy gap of bands usually gets closed and reopened in a nontrivial way accompanying a topological phase transition [9, 10]. For bosonic systems, SOC usually induces a shift of the energy minima from zero momentum to nonzero momentum with a number increase of the minima, as a result, the ground state of a spin-orbit coupled Bose-Einstein condensate (BEC) will have many possibilities and may exhibit new exotic phases of great interest [11–24].

Quantum magnetism, due to its fundamental importance in understanding many-body physics and its great potential applications in real life, is always one of the hottest fields in condensed matter physics [25, 26]. The simplest many-body model that exhibits quantum magnetism is the well-known Fermi-Hubbard model which plays a crucial role in understanding the high- T_c superconductor, however, as material systems always exhibit inevitable complexity, like defects, even though extensive efforts have been put in, a fully understanding of this simple model seems still far away. Therefore, to get a better understanding of the quantum magnetism in a controllable way, recently, several groups have put much efforts in engineering and observing magnetic order in cold atomic optical lattice systems [27–31]. These systems include both fermionic ones [29] and bosonic ones [27, 28, 30, 31]. As observing exchange-driven quantum magnetism of a fermionic system has been hindered by the required ultralow temperatures and entropies, currently most of the experiments are carried out in bosonic systems. For these bosonic systems, spin is usually mapped onto other physical quantities, like site occupation [27], momentum [31] or the local phase of a BEC [28, 30]. For the last mapping, as phase is not a quan-

tized number, such systems simulate classical magnetism.

In this work, we study a spin- $\frac{1}{2}$ BEC with a Rashba-like SOC loaded in a two-dimensional bipartite optical square lattice. Unlike previous studies that arbitrary small SOC will shift the energy minimum from zero momentum [11–24], here a shift of the energy minimum occurs only when the strength of SOC α reaches a critical value, *i.e.*, $\alpha > \alpha_c$. Furthermore, before and after the shift happen, the minima positions are fixed and parameter-independent. As the minima are symmetric and located at some special points of the Brillouin zone, there can exist some special scattering terms with total momentum equal to the reciprocal lattice vector \mathbf{G} , consequently, it is found that: (i) the ground state of the system always favors a coherent BEC instead of a fragmented BEC, (ii) with phase coherence guaranteed, the ground state always exhibits large degeneracy even in the appearance of interaction, (iii) with fixed parameters, all degenerate ground states correspond to the same spin configuration, (iv) most importantly, an *antiferromagnetic order of quantum nature* emerges when $\alpha > \alpha_c$ and interspin interaction is larger than intraspin interaction.

Theoretical model.—The lattice model we consider in this work is given as

$$\begin{aligned}
 H &= H_0 + H_{int} \\
 H_0 &= -\frac{t}{2} \sum_{\langle i,j \rangle, \sigma} (\hat{a}_{i\sigma}^\dagger \hat{b}_{j\sigma} + h.c.) - \Delta\mu \sum_{i \in A, \sigma} \hat{a}_{i\sigma}^\dagger \hat{a}_{i\sigma} + \\
 &\quad \Delta\mu \sum_{i \in B, \sigma} \hat{b}_{i\sigma}^\dagger \hat{b}_{i\sigma} + \left\{ \sum_{i \in A} \left[\frac{\alpha}{2} \hat{a}_{i,\uparrow}^\dagger (\hat{b}_{i+\hat{x},\downarrow} - \hat{b}_{i-\hat{x},\downarrow}) \right. \right. \\
 &\quad \left. \left. + \frac{i\alpha}{2} \hat{a}_{i,\uparrow}^\dagger (\hat{b}_{i+\hat{y},\downarrow} - \hat{b}_{i-\hat{y},\downarrow}) + h.c. \right] - [\hat{a} \longleftrightarrow \hat{b}] \right\} \\
 H_{int} &= \sum_{i \in A, \beta\gamma} U_{\beta\gamma, A} \hat{n}_{i\beta} \hat{n}_{i\gamma} + \sum_{i \in B, \beta\gamma} U_{\beta\gamma, B} \hat{n}_{i\beta} \hat{n}_{i\gamma} \\
 &= \sum_{i \in A} \left[\frac{c_{0,A}}{2} \hat{n}_i^2 + \frac{c_{2,A}}{2} \hat{S}_{z,i}^2 \right] + [A \longleftrightarrow B], \quad (1)
 \end{aligned}$$

where t denotes the nearest-neighbor hopping amplitude, $\Delta\mu$ denotes the staggered potential, and α denotes the

strength of spin-orbit coupling. $U_{\beta\gamma,A}$ and $U_{\beta\gamma,B}$ denote the strength of the interaction at sublattices A and B , respectively. σ , β and γ denote the two spin degrees $\{\uparrow, \downarrow\}$. $n_{i \in A, \beta} = \hat{a}_{i\beta}^\dagger \hat{a}_{i\beta}$ and $n_{i \in B, \beta} = \hat{b}_{i\beta}^\dagger \hat{b}_{i\beta}$ are the particle number operators for spin β and corresponding to sublattice A and B , respectively. $\hat{n}_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\hat{S}_{z,i} = n_{i,\uparrow} - n_{i,\downarrow}$. Without loss of generality, we assume $U_{\uparrow\uparrow,A(B)} = U_{\downarrow\downarrow,A(B)}$ and we use $U_{1,A(B)}$ to denote both of them. For $U_{\uparrow\downarrow,A(B)}$, we use $U_{2,A(B)}$ to denote it. Based on these, $c_{0,A(B)} = (U_{1,A(B)} + U_{2,A(B)})$, $c_{2,A(B)} = (U_{1,A(B)} - U_{2,A(B)})$, and the sign of $c_{2,A}$ and $c_{2,B}$ are the same.

By using a Fourier transformation, the Hamiltonian without interaction under the representation $\Phi_k = (\hat{a}_{k\uparrow}, \hat{b}_{k\downarrow}, \hat{b}_{k\uparrow}, \hat{a}_{k\downarrow})^T$ is given as

$$\mathcal{H}_0(k) = \epsilon_k \tau_x - \Delta \mu \sigma_z \tau_z + \Lambda_k \tau_z, \quad (2)$$

where $\epsilon_k = -t(\cos(k_x a) + \cos(k_y a))$ corresponds to the kinetic term, $\Lambda_k = \alpha(\sin(k_x a)\sigma_y - \sin(k_y a)\sigma_x)$ is the SOC which has a Rashba form. Note $\{\epsilon_k \tau_x, \Lambda_k \tau_z\} = 0$, this is different from the usual situation where kinetic term is commutative with the SOC term. As we will see, this difference induces quite different physical results. By making a transformation of the representation: $\tilde{\Phi}_k = (\hat{\alpha}_{1k}, \hat{\alpha}_{2k}, \hat{\beta}_{1k}, \hat{\beta}_{2k})^T = U(k)\Phi_k$ (see Supplementary Materials), the Hamiltonian (2) is diagonalized as

$$H_0 = \sum_k \left[-E_k(\hat{\alpha}_{1k}^\dagger \hat{\alpha}_{1k} + \hat{\alpha}_{2k}^\dagger \hat{\alpha}_{2k}) + E_k(\hat{\beta}_{1k}^\dagger \hat{\beta}_{1k} + \hat{\beta}_{2k}^\dagger \hat{\beta}_{2k}) \right], \quad (3)$$

where

$$E(k) = \sqrt{(\Delta \mu)^2 + \epsilon_k^2 + \alpha^2(\sin^2(k_x a) + \sin^2(k_y a))}, \quad (4)$$

the spectra have double degeneracy due to time-reversal symmetry: $\sigma_x \tau_x \mathcal{H}_0(k) \tau_x \sigma_x = \mathcal{H}_0^*(-k)$. For half-filling fermionic case with chemical potential $\mu = 0$, $\mathcal{H}_0(k)$ also holds particle-hole symmetry: $\sigma_x \tau_z \mathcal{H}_0(k) \tau_z \sigma_x = -\mathcal{H}_0^*(-k)$, and chiral symmetry: $\tau_y \mathcal{H}_0(k) \tau_y = -\mathcal{H}_0(k)$, therefore, it belongs to the BDI-class [9, 10, 32]. Such spin-orbit coupled system in one dimension under certain condition can exhibit nontrivial topological properties [33]. However, in this work we focus on a bosonic system where μ is always nonzero, what we concern is the lower band's minima where the bosons will be condensed, instead of the band gap in the fermionic case.

For bosons at low temperature, they will be condensed at the energy minima (we consider $T = 0$ in this work). Usually, there is only one minimum which is located at $\mathbf{k}_0 = 0$. However, from Eq.(4) or more directly from Fig.1, it is found that for this model, when $\alpha < \sqrt{2}t$, there are two minima which are stably located at $\mathbf{k}_0 = 0$ and $\mathbf{k}_\pi = (\pi/a, \pi/a)$, and when $\alpha > \sqrt{2}t$, there are four degenerate minima stably located at $\mathbf{Q}_1 = (\pi/2a, \pi/2a)$, $\mathbf{Q}_2 = (-\pi/2a, -\pi/2a)$, $\mathbf{Q}_3 = (\pi/2a, -\pi/2a)$, $\mathbf{Q}_4 = (-\pi/2a, \pi/2a)$. Increasing the strength of SOC α across

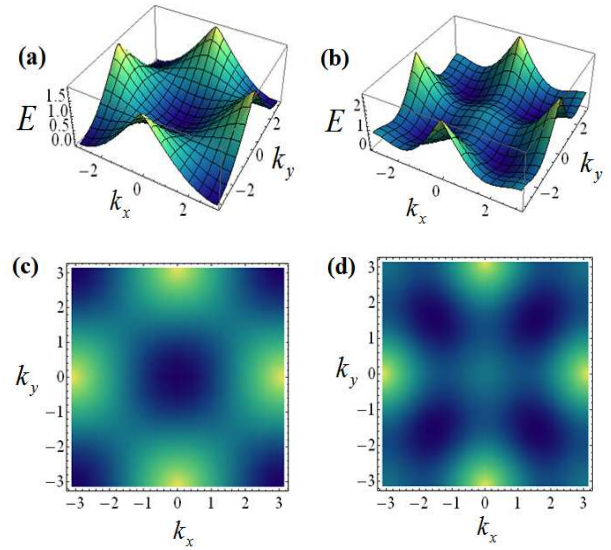


FIG. 1: (color online) (a)(b) Energy spectra correspond to Eq.(4). Parameters: we set $t = 1$ as the energy unit, and $a = 1$ as the length unit. (a)(c) $\Delta \mu = 0.1$, $\alpha = 1 < \alpha_c$. (b)(d) $\Delta \mu = 0.1$, $\alpha = 2 > \alpha_c$. (c) is the density plot of (a), and (d) is the density plot of (b). The deep color regions correspond to the energy minima.

the critical value $\alpha_c = \sqrt{2}t$, the minimum where the bosons are condensed will be shifted. As we will see, the shift is nontrivial, it not only directly alters the ground states, but also can establish an *antiferromagnetic* order in the condensate.

$\alpha < \alpha_c$, *two minima case*.— When $\alpha < \alpha_c$, to determine which minimum the bosons are condensed at, we introduce the wave functions which correspond to a fragmented and a coherent condensate, respectively, as [15]

$$\begin{aligned} |\Psi_f\rangle &= \frac{1}{\sqrt{M}} (\alpha_{1\mathbf{k}_0}^\dagger)^{N_{10}} (\alpha_{1\mathbf{k}_\pi}^\dagger)^{N_{1\pi}} (\alpha_{2\mathbf{k}_0}^\dagger)^{N_{20}} (\alpha_{2\mathbf{k}_\pi}^\dagger)^{N_{2\pi}} |0\rangle, \\ |\Psi_c\rangle &= \frac{1}{\sqrt{\Omega}} \{ \lambda_1 \hat{\alpha}_{1\mathbf{k}_0}^\dagger + e^{i\phi_1} \lambda_2 \hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \}^{N_1} \\ &\quad \{ \lambda_3 \hat{\alpha}_{2\mathbf{k}_0}^\dagger + e^{i\phi_2} \lambda_4 \hat{\alpha}_{2\mathbf{k}_\pi}^\dagger \}^{N_2} |0\rangle, \end{aligned} \quad (5)$$

where $M = N_{10}! N_{1\pi}! N_{20}! N_{2\pi}!$, $\lambda_1 = \sqrt{N_{10}/N_1}$, $\lambda_2 = \sqrt{N_{1\pi}/N_1}$, $\lambda_3 = \sqrt{N_{20}/N_2}$, $\lambda_4 = \sqrt{N_{2\pi}/N_2}$, $\Omega = N_1! N_2!$. The particle number partition $(N_{10}, N_{1\pi})$ and $(N_{20}, N_{2\pi})$ satisfy the constraint: $N_{10} + N_{1\pi} = N_1$, $N_{20} + N_{2\pi} = N_2$. Without loss of generality, we assume $N_1 = N_2 = N/2$ where N is the total particle number in the condensate.

Since the kinetic energy of a condensate is negligible, we only need to consider the interaction energy $\langle \Psi | H_{int} | \Psi \rangle$. Based on the wave function of a frag-

mented condensate, the expression is given as [34]

$$\begin{aligned}
\langle \Psi_f | H_{int} | \Psi_f \rangle &= [U_{1,A} N_1 (N_1 - 1) + U_{1,A} N_2 (N_2 - 1) \\
&\quad + 2U_{2,A} N_1 N_2] \cos^4(\theta/2) + [U_{1,B} N_1 (N_1 - 1) \\
&\quad + U_{1,B} N_2 (N_2 - 1) + 2U_{2,B} N_1 N_2] \sin^4(\theta/2) \\
&\quad + 2[U_{1,A} (N_{10} N_{1\pi} + N_{20} N_{2\pi}) \cos^4(\theta/2) \\
&\quad + U_{1,B} (N_{10} N_{1\pi} + N_{20} N_{2\pi}) \sin^4(\theta/2)] \\
&= E_s + E_{Fock}, \tag{6}
\end{aligned}$$

where E_s is the sum of the terms in the first three lines, and E_{Fock} is the sum of the terms in the fourth and fifth lines. Due to the Fock terms, the fragmented condensate, compared to a *single condensate* (either $N_0 = 0$ or $N_\pi = 0$) which only has energy E_s , always costs more energy and therefore is unfavored. Based on the wave function of a coherent condensate,

$$\begin{aligned}
\langle \Psi_c | H_{int} | \Psi_c \rangle &= \langle \Psi_f | H_{int} | \Psi_f \rangle + 2[U_{1,A} N_{10} N_{1\pi} \\
&\quad \times \frac{(N_1 - 1)}{N_1} \cos(2\phi_1) + U_{1,A} N_{20} N_{2\pi} \frac{(N_2 - 1)}{N_2} \cos(2\phi_2) \\
&\quad + 4U_{2,A} \sqrt{N_{10} N_{1\pi} N_{20} N_{2\pi}} \cos(\phi_1) \cos(\phi_2)] \cos^4(\theta/2) \\
&\quad + 2[U_{1,B} N_{10} N_{1\pi} \frac{(N_1 - 1)}{N_1} \cos(2\phi_1) + U_{2,B} N_{20} N_{2\pi} \\
&\quad \times \frac{(N_2 - 1)}{N_2} \cos(2\phi_2) + 4U_{2,B} \sqrt{N_{10} N_{1\pi} N_{20} N_{2\pi}} \\
&\quad \times \cos(\phi_1) \cos(\phi_2)] \sin^4(\theta/2), \tag{7}
\end{aligned}$$

where $\theta = \arctan(2t/\Delta\mu)$. Compared $\langle \Psi_c | H_{int} | \Psi_c \rangle$ to $\langle \Psi_f | H_{int} | \Psi_f \rangle$, the additional terms appearing in Eq.(7) is due to the fact that the system is a lattice one, therefore, unlike the continue case, such terms like $\hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \hat{\alpha}_{1\mathbf{k}_0} \hat{\alpha}_{1\mathbf{k}_0}$ and $\hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \hat{\alpha}_{2\mathbf{k}_\pi}^\dagger \hat{\alpha}_{2\mathbf{k}_0} \hat{\alpha}_{1\mathbf{k}_0}$ are allowed because $2(\mathbf{k}_\pi - \mathbf{k}_0) = \mathbf{G}$, where \mathbf{G} is the reciprocal vector. The appearance of these additional terms makes the *coherent condensate always more favored than the fragmented condensate* since $\langle \Psi_c | H_{int} | \Psi_c \rangle$ can always be made to be smaller than $\langle \Psi_f | H_{int} | \Psi_f \rangle$ by tuning the phase ϕ_1 and ϕ_2 . Therefore, to determine the ground state, what we need to do is to minimize $\langle \Psi_c | H_{int} | \Psi_c \rangle$.

As N is generally large, $(N_i - 1)/N_i$ can be taken as 1. It is found that when $U_2 < U_1$, $\langle \Psi_c | H_{int} | \Psi_c \rangle$ takes the same minimum value E_s for arbitrary particle number partition if the phases ϕ_1 and ϕ_2 are locked to $\{(n + \frac{1}{2})\pi, n \in \mathbb{Z}\}$. Therefore, the degeneracy of the ground state is very large ($\propto N^2$), these degenerate ground states can be written compactly as

$$\begin{aligned}
|\Psi_g\rangle &= \frac{1}{\sqrt{\Omega}} \{ \lambda_1 \hat{\alpha}_{1\mathbf{k}_0}^\dagger \pm i \lambda_2 \hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \}^{N_1} \\
&\quad \{ \lambda_3 \hat{\alpha}_{2\mathbf{k}_0}^\dagger \pm i \lambda_4 \hat{\alpha}_{2\mathbf{k}_\pi}^\dagger \}^{N_2} |0\rangle. \tag{8}
\end{aligned}$$

When $U_2 > U_1$, the ground state wave function keeps its form in Eq.(8), but to reach the ground state, the system will undergo a phase separation. Besides, there emerges two new possible ground states where $N_{10} =$

$N_{1\pi} = N_{20} = N_{2\pi} = N/4$ and ϕ_1 and ϕ_2 are either given as $\phi_1 = 0$ and $\phi_2 = \pi$ or $\phi_1 = \pi$ and $\phi_2 = 0$. The two phases turn out to be locked to each other. The two new possible ground state wave functions can be written as

$$|\tilde{\Psi}_g\rangle = \frac{1}{\sqrt{2N\Omega}} \{ \hat{\alpha}_{1\mathbf{k}_0}^\dagger \pm \hat{\alpha}_{1\mathbf{k}_\pi}^\dagger \}^{N_1} \{ \hat{\alpha}_{2\mathbf{k}_0}^\dagger \mp \hat{\alpha}_{2\mathbf{k}_\pi}^\dagger \}^{N_2} |0\rangle. \tag{9}$$

Although the ground state has very large degeneracy, the system in real space will only exhibit two kinds of spin-configurations. In order to show this, we write down the spinor wave function corresponding to the condensate in real space,

$$\vec{\varphi}(\mathbf{r}) = \sqrt{n_0} [(a_1 \vec{e}_1 + a_2 \vec{e}_2) e^{i\mathbf{k}_\pi \cdot \mathbf{r}} + (a_3 \vec{e}_3 + a_4 \vec{e}_4)], \tag{10}$$

where $n_0 = N/N_T$ is the condensation density with N_T the number of lattice sites, $\vec{\varphi} = [\varphi_{A,\uparrow}, \varphi_{B,\downarrow}, \varphi_{B,\uparrow}, \varphi_{A,\downarrow}]^T$, $\vec{e}_1 = [\chi_1, 0, -\chi_2, 0]^T$, $\vec{e}_2 = [0, -\chi_2, 0, \chi_1]^T$, $\vec{e}_3 = [\chi_1, 0, \chi_2, 0]^T$, $\vec{e}_4 = [0, \chi_2, 0, \chi_1]^T$, with $\chi_1 = \cos(\theta/2)$, $\chi_2 = \sin(\theta/2)$, $\theta = \arctan(2t/\Delta\mu)$. a_i are complex coefficients which satisfy $|a_1|^2 + |a_3|^2 = |a_2|^2 + |a_4|^2 = 1$ and are determined by minimizing the energy functional

$$\begin{aligned}
\varepsilon &= \sum_{i \in A} [\frac{c_{0,A}}{2} (|\varphi_{i,\uparrow}|^2 + |\varphi_{i,\downarrow}|^2)^2 + \frac{c_{2,A}}{2} (|\varphi_{i,\uparrow}|^2 - |\varphi_{i,\downarrow}|^2)^2] \\
&\quad + (A \longleftrightarrow B). \tag{11}
\end{aligned}$$

(7) From Eq.(10), it is direct to obtain

$$\begin{aligned}
|\varphi_{i \in A, \uparrow}|^2 &= n_0 \chi_1^2 (1 + 2|a_1||a_3| \cos[\frac{\pi(x_i + y_i)}{a} + \phi_1]) \xi_1, \\
|\varphi_{i \in B, \uparrow}|^2 &= n_0 \chi_2^2 (1 - 2|a_1||a_3| \cos[\frac{\pi(x_i + y_i)}{a} + \phi_1]) \xi_2, \\
|\varphi_{i \in A, \downarrow}|^2 &= n_0 \chi_1^2 (1 + 2|a_2||a_4| \cos[\frac{\pi(x_i + y_i)}{a} + \phi_2]) \xi_1, \\
|\varphi_{i \in B, \downarrow}|^2 &= n_0 \chi_2^2 (1 - 2|a_2||a_4| \cos[\frac{\pi(x_i + y_i)}{a} + \phi_2]) \xi_2, \tag{12}
\end{aligned}$$

where $\xi_1 = [(-1)^{x_i/a} + (-1)^{y_i/a}]^2/4$, $\xi_2 = [(-1)^{x_i/a} - (-1)^{y_i/a}]^2/4$, here we have made a choice that sublattices A correspond to that x_i/a and y_i/a are simultaneously even or odd. When $U_2 < U_1$, i.e., $c_{2,A(B)} > 0$, it is not hard to obtain that when $|\varphi_{i \in A, \uparrow}|^2 = |\varphi_{i \in A, \downarrow}|^2 = n_0 \chi_1^2 \xi_1$, $|\varphi_{i \in B, \uparrow}|^2 = |\varphi_{i \in B, \downarrow}|^2 = n_0 \chi_2^2 \xi_2$, the energy functional (11) take its minimum value. The above condition is satisfied for arbitrary a_i if ϕ_1 and ϕ_2 are locked to $\{(n + \frac{1}{2})\pi, n \in \mathbb{Z}\}$. We can find that the same conclusion as the one above Eq.(8) is reached. Therefore, these degenerate ground states described by Eq.(8) all correspond to a *spin-balanced* or *paramagnetic* condensate, shown in Fig.2(a). When $U_2 > U_1$, $c_{2,A(B)} < 0$, it is found that the case with $a_1 = a_2 = a_3 = a_4 = 1/2$, which corresponds to $N_{10} = N_{1\pi} = N_{20} = N_{2\pi} = N/2$, the phases should be given as $\{\phi_1(0 < x_i < L_x/2, y_i) = 0 \text{ or } \pi, \phi_2(0 < x_i < L_x/2, y_i) = \pi \text{ or } 0, \delta\phi = \pi \text{ mod } 2\pi\}$ and $\{\phi_1(L_x/2 < x_i < L_x, y_i) = \pi - \phi_1(0 < x_i < L_x/2, y_i), \phi_2(L_x/2 < x_i < L_x, y_i) = \pi - \phi_2(0 < x_i < L_x/2, y_i)\}$ (we

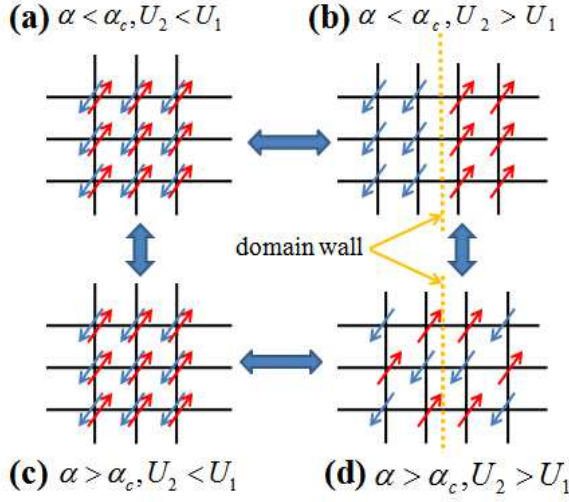


FIG. 2: (color online) Spin configurations correspond to different parameter regions. (a)(c) paramagnetic configuration, (b) ferromagnetic configuration, (d) antiferromagnetic configuration. The domain walls in (b)(d) are a result of number conservation for each spin.

have assumed $L_y > L_x$. Other phase configurations always exhibit more stronger suppression of hopping, and therefore, are not favored in energy). From Eq.(12), we can obtain that this phase configuration corresponds to a phase-separation *ferromagnetic* condensate, shown in Fig.2(b). Therefore, when $U_2 > U_1$, all degenerate ground states corresponds to a *ferromagnetic* condensate.

$\alpha > \alpha_c$, *four minima case*.— This case is our most interested case. When $\alpha > \alpha_c$, there are four energy minima $\mathbf{Q}_{1,2,3,4}$. Similar to the two minima case, we introduce two wave functions which correspond to a fragmented and a coherent condensate, respectively, as

$$\begin{aligned}
 |\tilde{\Psi}_f\rangle &= \frac{1}{\sqrt{\tilde{M}}} (\alpha_{1\mathbf{Q}_1}^\dagger)^{N_{11}} (\alpha_{1\mathbf{Q}_2}^\dagger)^{N_{12}} (\alpha_{1\mathbf{Q}_3}^\dagger)^{N_{13}} (\alpha_{1\mathbf{Q}_4}^\dagger)^{N_{14}} \\
 &\quad (\alpha_{2\mathbf{Q}_1}^\dagger)^{N_{21}} (\alpha_{2\mathbf{Q}_2}^\dagger)^{N_{22}} (\alpha_{2\mathbf{Q}_3}^\dagger)^{N_{23}} (\alpha_{2\mathbf{Q}_4}^\dagger)^{N_{24}} |0\rangle, \\
 |\tilde{\Psi}_c\rangle &= \frac{1}{\sqrt{\tilde{\Omega}}} \{ \lambda_{11} \alpha_{1\mathbf{Q}_1}^\dagger + \lambda_{12} e^{i\varphi_{1,2}} \alpha_{1\mathbf{Q}_2}^\dagger + \lambda_{13} e^{i\varphi_{1,3}} \alpha_{1\mathbf{Q}_3}^\dagger \\
 &\quad + \lambda_{14} e^{i\varphi_{1,4}} \alpha_{1\mathbf{Q}_4}^\dagger \}^{N_1} \{ \lambda_{21} \alpha_{2\mathbf{Q}_1}^\dagger + \lambda_{22} e^{i\varphi_{2,2}} \alpha_{2\mathbf{Q}_2}^\dagger \\
 &\quad + \lambda_{23} e^{i\varphi_{2,3}} \alpha_{2\mathbf{Q}_3}^\dagger + \lambda_{24} e^{i\varphi_{2,4}} \alpha_{2\mathbf{Q}_4}^\dagger \}^{N_2} |0\rangle, \quad (13)
 \end{aligned}$$

where $\tilde{M} = \prod_{i=1}^4 N_{1i}! N_{2i}!$, $\lambda_{ij} = \sqrt{N_{ij}/N_i}$. Similarly, it is direct to obtain that

$$\begin{aligned}
 \langle \tilde{\Psi}_f | H_{int} | \tilde{\Psi}_f \rangle &= [U_{1,A} N_1 (N_1 - 1) + U_{1,A} N_2 (N_2 - 1) \\
 &\quad + 2U_{2,A} N_1 N_2] \cos^4(\tilde{\theta}/2) + [U_{1,B} N_1 (N_1 - 1) \\
 &\quad + U_{1,B} N_2 (N_2 - 1) + 2U_{2,B} N_1 N_2] \sin^4(\tilde{\theta}/2) + \\
 &\quad 2 \sum_{i=1}^4 [U_{1,A} N_{1i} N_{1j} \cos^4(\frac{\tilde{\theta}}{2}) + U_{1,B} N_{2i} N_{2j} \sin^4(\frac{\tilde{\theta}}{2})] \\
 &= \tilde{E}_s + \tilde{E}_{Fock}, \quad (14)
 \end{aligned}$$

where the terms in the fourth line correspond to \tilde{E}_{Fock} , and $\tilde{\theta} = \arctan(\sqrt{2}\alpha/\Delta\mu)$. As $\tilde{\theta} > \theta$ and $U_A > U_B$ (sublattices B will be shallower than A), it is not hard to see that \tilde{E}_s is smaller than E_s , however, this decrease is quite small at the neighborhood of the critical point, $\alpha = \alpha_c$, if $N_{1j} = N_1/4$ and $N_{2j} = N_2/4$ for arbitrary j , \tilde{E}_{Fock} is approximately equal to $3E_{Fock}/2$. This suggests that a more fragmented condensate costs more energy.

The concrete form of $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle$ is very tedious and is given explicitly in the Supplementary Materials. Based on $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle$, it is also found that the ground state has large degeneracy. When $U_2 < U_1$, the bosons can be condensed at: one of the minima \mathbf{Q}_i , or two time-reversal-partner minima $\{\mathbf{Q}_i, -\mathbf{Q}_i\}$, or four minima simultaneously with $N_{1j} = N_1/4$ and $N_{2j} = N_2/4$ for arbitrary j . The first two cases can be described by a wave function similar to Eq.(8), for the last one, the ground state wave function is given as

$$\begin{aligned}
 |\tilde{\Psi}_g\rangle &= \frac{1}{\sqrt{4^{N\Omega}}} \{ (\hat{\alpha}_{1\mathbf{Q}_1}^\dagger - \hat{\alpha}_{1\mathbf{Q}_2}^\dagger) \pm i(\hat{\alpha}_{1\mathbf{Q}_3}^\dagger + \hat{\alpha}_{1\mathbf{Q}_4}^\dagger) \}^{N_1} \\
 &\quad \{ (\hat{\alpha}_{2\mathbf{Q}_1}^\dagger - \hat{\alpha}_{2\mathbf{Q}_2}^\dagger) \pm i(\hat{\alpha}_{2\mathbf{Q}_3}^\dagger + \hat{\alpha}_{2\mathbf{Q}_4}^\dagger) \}^{N_2} |0\rangle \quad (15)
 \end{aligned}$$

When $U_2 > U_1$, it is found that the degeneracy is greatly reduced, there are only eight possible degenerate ground states which can be written compactly as

$$\begin{aligned}
 |\tilde{\Psi}_g\rangle &= \frac{1}{\sqrt{2^{N\Omega}}} \{ \gamma_1 (\hat{\alpha}_{1\mathbf{Q}_1}^\dagger \pm \hat{\alpha}_{1\mathbf{Q}_2}^\dagger) + \gamma_2 (\hat{\alpha}_{1\mathbf{Q}_3}^\dagger \pm \hat{\alpha}_{1\mathbf{Q}_4}^\dagger) \}^{N_1} \\
 &\quad \{ \gamma_3 (\hat{\alpha}_{2\mathbf{Q}_1}^\dagger \mp \hat{\alpha}_{2\mathbf{Q}_2}^\dagger) + \gamma_4 (\hat{\alpha}_{2\mathbf{Q}_3}^\dagger \mp \hat{\alpha}_{2\mathbf{Q}_4}^\dagger) \}^{N_2} |0\rangle \quad (16)
 \end{aligned}$$

where $\gamma_{1,2,3,4}$ only take two values $\{0, 1\}$ and $\gamma_2 = 1 - \gamma_1$, $\gamma_4 = 1 - \gamma_3$. Eq.(16) suggests that for each degree, $\hat{\alpha}_1$ or $\hat{\alpha}_2$, the bosons can only choose one pair of the time-reversal-partner minima to condense.

Similar to the two minima case, although the degeneracy of the ground states are large, there are also only two kinds of spin configurations. Following the previous procedures, we first write down the spinor wave function corresponding to the condensate,

$$\begin{aligned}
 \vec{\varphi}(\mathbf{r}) &= \sqrt{n_0} [(b_1 \vec{u}_1 + b_2 \vec{u}_2) e^{i\mathbf{Q}_1 \cdot \mathbf{r}} + (b_3 \vec{u}_3 + b_4 \vec{u}_4) e^{i\mathbf{Q}_2 \cdot \mathbf{r}} \\
 &\quad + (b_5 \vec{u}_5 + b_6 \vec{u}_6) e^{i\mathbf{Q}_3 \cdot \mathbf{r}} + (b_7 \vec{u}_7 + b_8 \vec{u}_8) e^{i\mathbf{Q}_4 \cdot \mathbf{r}}] \quad (17)
 \end{aligned}$$

where $\vec{u}_1 = [\tilde{\chi}_1, \tilde{\chi}_2 e^{-i\pi/4}, 0, 0]^T$, $\vec{u}_2 = [0, 0, -\tilde{\chi}_2 e^{i\pi/4}, \tilde{\chi}_1]^T$, $\vec{u}_3 = [\tilde{\chi}_1, -\tilde{\chi}_2 e^{-i\pi/4}, 0, 0]^T$, $\vec{u}_4 = [0, 0, \tilde{\chi}_2 e^{i\pi/4}, \tilde{\chi}_1]^T$, $\vec{u}_5 = [\tilde{\chi}_1, -\tilde{\chi}_2 e^{i\pi/4}, 0, 0]^T$, $\vec{u}_6 = [0, 0, \tilde{\chi}_2 e^{-i\pi/4}, \tilde{\chi}_1]^T$, $\vec{u}_7 = [\tilde{\chi}_1, \tilde{\chi}_2 e^{i\pi/4}, 0, 0]^T$, $\vec{u}_8 = [0, 0, -\tilde{\chi}_2 e^{-i\pi/4}, \tilde{\chi}_1]^T$, with $\tilde{\chi}_1 = \cos(\tilde{\theta}/2)$, $\tilde{\chi}_2 = \sin(\tilde{\theta}/2)$. b_i are complex coefficients which satisfy $|b_1|^2 + |b_3|^2 + |b_5|^2 + |b_7|^2 = |b_2|^2 + |b_4|^2 + |b_6|^2 + |b_8|^2 = 1$ and are determined by minimizing Eq.(11).

Based on Eq.(17), the particle distribution can be directly obtained (see Supplementary Materials). It is direct to find that when $U_2 < U_1$, the degenerate ground states for the aforementioned three cases all correspond to a *paramagnetic* condensate, i.e., $|\varphi_{i \in A, \uparrow}|^2 =$

$|\varphi_{i \in A, \downarrow}|^2 = n_0 \chi_1^2 \xi_1$, $|\varphi_{i \in B, \uparrow}|^2 = |\varphi_{i \in B, \downarrow}|^2 = n_0 \chi_2^2 \xi_2$, shown in Fig.2(c). When $U_2 > U_1$, with the constraint of particle number conservation, it is found that the particle distribution corresponding to the ground states given in Eq.(16) should be: $\{|\varphi_{i \in A \uparrow}|^2 = 2n_0 \tilde{\chi}_1^2 \xi_1, |\varphi_{i \in A \downarrow}|^2 = 0, |\varphi_{i \in B \downarrow}|^2 = 2n_0 \tilde{\chi}_2^2 \xi_2, |\varphi_{i \in B \uparrow}|^2 = 0, \text{ and } |\varphi_{j \in A \uparrow}|^2 = 0, |\varphi_{j \in A \downarrow}|^2 = 2n_0 \tilde{\chi}_1^2 \xi_1, |\varphi_{j \in B \downarrow}|^2 = 0, |\varphi_{j \in B \uparrow}|^2 = 2n_0 \tilde{\chi}_2^2 \xi_2\}$, or $\{|\varphi_{i \in A \uparrow}|^2 = 0, |\varphi_{i \in A \downarrow}|^2 = 2n_0 \tilde{\chi}_1^2 \xi_1, |\varphi_{i \in B \downarrow}|^2 = 0, |\varphi_{i \in B \uparrow}|^2 = 2n_0 \tilde{\chi}_2^2 \xi_2, \text{ and } |\varphi_{j \in A \uparrow}|^2 = 2n_0 \tilde{\chi}_1^2 \xi_1, |\varphi_{j \in A \downarrow}|^2 = 0, |\varphi_{j \in B \downarrow}|^2 = 2n_0 \tilde{\chi}_2^2 \xi_2, |\varphi_{j \in B \uparrow}|^2 = 0\}$, with $0 < x_i < L_x/2$, $L_x/2 < x_j < L_x$, shown in Fig.2(d). Therefore, all ground states correspond to a condensate with *antiferromagnetic order of quantum nature* (quantum nature means that the site-magnetization away from the domain wall has only two possible values). The *antiferromagnetic order* is a direct result of the existence of the four degenerate separated minima $\mathbf{Q}_{1,2,3,4}$, which themselves are a result of the anticommutation relation $\{\epsilon_k \tau_x, \Lambda_k \tau_z\} = 0$. Therefore, The key to realize the interesting *antiferromagnetic order* is to realize the Rashba-like SOC, $\Lambda_k \tau_z$, which needs a non-Abelian gauge field currently beyond the realization ability of experiments. If SOC is as usual commutative with kinetic term, the momentum shift of the minima can reach the values of \mathbf{Q}_i only when α/t goes to infinite which is hard to realize. For general finite α/t , just like continuous systems [13, 16], the lattice system will exhibit site-dependent magnetization which is a classical quantity, but can not establish the *antiferromagnetic order* of quantum nature like here, which exists in a wide range of parameters.

Discussions and Conclusions.— Duo to the existence of scattering processes related to the reciprocal lattice vector, it is found that the ground states always favor a coherent condensate and always exhibit very large degeneracy. However, this conclusion should only be valid when the effect of quantum fluctuations is small and the phase keeps coherent. When phase coherence is lost (then the ground state energy is obtained by averaging the phases [35]), the degeneracy will be greatly reduced and the ground state is inclined to a *single* condensate. This crossover can be observed by time-of-flight experiments. As with fixed parameters, all ground states correspond to the same spin configuration, which suggests that the spin configurations are in fact more stable than the ground states. The spin configurations can be revealed by spin-dependent imaging techniques. The minima where the bosons are condensed and the shift of the minima when α goes across α_c can also be observed by time-of-flight experiments.

The coexistence of superfluidity and antiferromagnetic order in a cold atomic system, which are the most two important phases in high- T_c superconductors, opens a door to study their interplay in a controllable way.

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SUPPLEMENTARY MATERIALS

A. Interaction under new representation.

For Hamiltonian (1), by redefining a representation $\tilde{\Phi}_k = (\hat{\alpha}_{1k}, \hat{\alpha}_{2k}, \hat{\beta}_{1k}, \hat{\beta}_{2k})^T = U(k)\Phi_k$, where $U(k)$ is a 4×4 matrix with the form

$$U(k) = \begin{pmatrix} \frac{E(k)+\Delta\mu}{\mathcal{N}_1} & 0 & \frac{-E(k)+\Delta\mu}{\mathcal{N}_2} & 0 \\ -\frac{\epsilon_k}{\mathcal{N}_1} & \frac{A^*(k)}{\mathcal{N}_1} & -\frac{\epsilon_k}{\mathcal{N}_2} & \frac{A^*(k)}{\mathcal{N}_2} \\ -\frac{\epsilon_k}{\mathcal{N}_1} & \frac{A^*(k)}{\mathcal{N}_1} & -\frac{\epsilon_k}{\mathcal{N}_2} & \frac{A^*(k)}{\mathcal{N}_2} \\ 0 & \frac{E(k)+\Delta\mu}{\mathcal{N}_1} & 0 & \frac{-E(k)+\Delta\mu}{\mathcal{N}_2} \end{pmatrix}^{-1} \quad (18)$$

where $E(k) = \sqrt{(\Delta\mu)^2 + \epsilon_k^2 + \alpha^2(\sin^2(k_x a) + \sin^2(k_y a))}$, $A(k) = i\alpha \sin(k_x a) - \alpha \sin(k_y a)$, $\epsilon_k = -t(\cos(k_x a) + \cos(k_y a))$, $\mathcal{N}_1 = \sqrt{2E(k)(E(k) + \Delta\mu)}$, $\mathcal{N}_2 = \sqrt{2E(k)(E(k) - \Delta\mu)}$, then the Hamiltonian is diagonalized as

$$H_0 = \sum_k [-E(k)(\hat{\alpha}_{1k}^\dagger \hat{\alpha}_{1k} + \hat{\alpha}_{2k}^\dagger \hat{\alpha}_{2k}) + E(k)(\hat{\beta}_{1k}^\dagger \hat{\beta}_{1k} + \hat{\beta}_{2k}^\dagger \hat{\beta}_{2k})]. \quad (19)$$

In the following, we set $\lambda_1(k) = \frac{E(k)+\Delta\mu}{\mathcal{N}_1}$, $\lambda_2(k) = \frac{-E(k)+\Delta\mu}{\mathcal{N}_2}$, $\lambda_3 = \frac{A(k)}{\mathcal{N}_1}$, $\lambda_4 = \frac{\epsilon_k}{\mathcal{N}_1}$, $\lambda_5 = \frac{A(k)}{\mathcal{N}_2}$, $\lambda_6 = \frac{\epsilon_k}{\mathcal{N}_2}$. Then $\hat{a}_{k\uparrow} = \lambda_1(k)\hat{\alpha}_{1k} + \lambda_2(k)\hat{\beta}_{1k}$, $\hat{a}_{k\downarrow} = \lambda_1(k)\hat{\alpha}_{2k} + \lambda_2(k)\hat{\beta}_{2k}$, $\hat{b}_{k\downarrow} = -(\lambda_3(k)\hat{\alpha}_{1k} + \lambda_4(k)\hat{\alpha}_{2k} + \lambda_5(k)\hat{\beta}_{1k} + \lambda_6(k)\hat{\beta}_{2k})$, $\hat{b}_{k\uparrow} = -(\lambda_4(k)\hat{\alpha}_{1k} - \lambda_3(k)\hat{\alpha}_{2k} + \lambda_6(k)\hat{\beta}_{1k} - \lambda_5(k)\hat{\beta}_{2k})$.

Under this representation, the form of the interaction will turn out to be very complicated. The concrete interaction forms for sublattices A are

$$\begin{aligned} & g_{1A} \sum_{k_1, k_2, k_3, k_4} \hat{a}_{k_1\uparrow}^\dagger \hat{a}_{k_2\uparrow}^\dagger \hat{a}_{k_3\uparrow} \hat{a}_{k_4\uparrow} \\ &= g_{1A} \sum_{k_1, k_2, k_3, k_4} (\lambda_1^*(k_1)\hat{\alpha}_{1k_1}^\dagger + \lambda_2^*(k_1)\hat{\beta}_{1k_1}^\dagger)(\lambda_1^*(k_2)\hat{\alpha}_{1k_2}^\dagger + \lambda_2^*(k_2)\hat{\beta}_{1k_2}^\dagger)(\lambda_1(k_3)\hat{\alpha}_{1k_3} + \lambda_2(k_3)\hat{\beta}_{1k_3})(\lambda_1(k_4)\hat{\alpha}_{1k_4} + \lambda_2(k_4)\hat{\beta}_{1k_4}) \\ &= g_{1A} \sum_{k_1, k_2, k_3, k_4} [\lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + 2\lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\beta}_{1k_4} \\ &\quad + \lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\beta}_{1k_3} \hat{\beta}_{1k_4} + 2\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} \\ &\quad + 4\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\beta}_{1k_4} + 2\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\beta}_{1k_3} \hat{\beta}_{1k_4} \\ &\quad + \lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\beta}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + 2\lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\beta}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\beta}_{1k_4} \\ &\quad + \lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\beta}_{1k_1}^\dagger \hat{\beta}_{1k_2}^\dagger \hat{\beta}_{1k_3} \hat{\beta}_{1k_4}], \\ & g_{1A} \sum_{k_1, k_2, k_3, k_4} \hat{a}_{k_1\downarrow}^\dagger \hat{a}_{k_2\downarrow}^\dagger \hat{a}_{k_3\downarrow} \hat{a}_{k_4\downarrow} \\ &= g_{1A} \sum_{k_1, k_2, k_3, k_4} (\lambda_1^*(k_1)\hat{\alpha}_{2k_1}^\dagger + \lambda_2^*(k_1)\hat{\beta}_{2k_1}^\dagger)(\lambda_1^*(k_2)\hat{\alpha}_{2k_2}^\dagger + \lambda_2^*(k_2)\hat{\beta}_{2k_2}^\dagger)(\lambda_1(k_3)\hat{\alpha}_{2k_3} + \lambda_2(k_3)\hat{\beta}_{2k_3})(\lambda_1(k_4)\hat{\alpha}_{2k_4} + \lambda_2(k_4)\hat{\beta}_{2k_4}) \\ &= g_{1A} \sum_{k_1, k_2, k_3, k_4} [\lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} + 2\lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\beta}_{2k_4} \\ &\quad + \lambda_1^*(k_1)\lambda_1^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\beta}_{2k_3} \hat{\beta}_{2k_4} + 2\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} \\ &\quad + 4\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\beta}_{2k_4} + 2\lambda_1^*(k_1)\lambda_2^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\beta}_{2k_3} \hat{\beta}_{2k_4} \\ &\quad + \lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_1(k_4)\hat{\beta}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} + 2\lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_1(k_3)\lambda_2(k_4)\hat{\beta}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\beta}_{2k_4} \\ &\quad + \lambda_2^*(k_1)\lambda_2^*(k_2)\lambda_2(k_3)\lambda_2(k_4)\hat{\beta}_{2k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\beta}_{2k_3} \hat{\beta}_{2k_4}], \end{aligned}$$

$$\begin{aligned}
& 2g_{12A} \sum_{k_1, k_2, k_3, k_4} \hat{a}_{k_1\downarrow}^\dagger \hat{a}_{k_2\downarrow}^\dagger \hat{a}_{k_3\downarrow} \hat{a}_{k_4\downarrow} \\
&= g_{12A} \sum_{k_1, k_2, k_3, k_4} (\lambda_1^*(k_1) \hat{\alpha}_{1k_1}^\dagger + \lambda_2^*(k_1) \hat{\beta}_{1k_1}^\dagger) (\lambda_1^*(k_2) \hat{\alpha}_{2k_2}^\dagger + \lambda_2^*(k_2) \hat{\beta}_{2k_2}^\dagger) (\lambda_1(k_3) \hat{\alpha}_{2k_3} + \lambda_2(k_3) \hat{\beta}_{2k_3}) (\lambda_1(k_4) \hat{\alpha}_{1k_4} + \lambda_2(k_4) \hat{\beta}_{1k_4}) \\
&= 2g_{12A} \sum_{k_1, k_2, k_3, k_4} [\lambda_1^*(k_1) \lambda_1^*(k_2) \lambda_1(k_3) \lambda_1(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4} + \lambda_1^*(k_1) \lambda_1^*(k_2) \lambda_1(k_3) \lambda_2(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger (\hat{\alpha}_{2k_3} \hat{\beta}_{1k_4} + \hat{\alpha}_{1k_3} \hat{\beta}_{2k_4}) \\
&\quad + \lambda_1^*(k_1) \lambda_1^*(k_2) \lambda_2(k_3) \lambda_2(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\beta}_{2k_3} \hat{\beta}_{1k_4} + \lambda_1^*(k_1) \lambda_2^*(k_2) \lambda_1(k_3) \lambda_1(k_4) (\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger + \hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{1k_2}^\dagger) \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4} \\
&\quad + \lambda_1^*(k_1) \lambda_2^*(k_2) \lambda_1(k_3) \lambda_2(k_4) (\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger + \hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{1k_2}^\dagger) (\hat{\alpha}_{2k_3} \hat{\beta}_{1k_4} + \hat{\alpha}_{1k_3} \hat{\beta}_{2k_4}) + \lambda_1^*(k_1) \lambda_2^*(k_2) \lambda_2(k_3) \lambda_2(k_4) \\
&\quad (\hat{\alpha}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger + \hat{\alpha}_{2k_1}^\dagger \hat{\beta}_{1k_2}^\dagger) \hat{\beta}_{2k_3} \hat{\beta}_{2k_4} + \lambda_2^*(k_1) \lambda_2^*(k_2) \lambda_1(k_3) \lambda_1(k_4) \hat{\beta}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4} \\
&\quad + \lambda_2^*(k_1) \lambda_2^*(k_2) \lambda_1(k_3) \lambda_2(k_4) \hat{\beta}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger (\hat{\alpha}_{1k_3} \hat{\beta}_{2k_4} + \hat{\alpha}_{2k_3} \hat{\beta}_{1k_4}) + \lambda_2^*(k_1) \lambda_2^*(k_2) \lambda_2(k_3) \lambda_2(k_4) \hat{\beta}_{1k_1}^\dagger \hat{\beta}_{2k_2}^\dagger \hat{\beta}_{2k_3} \hat{\beta}_{1k_4}],
\end{aligned}$$

where the four momentums $\mathbf{k}_{1,2,3,4}$ for summation belong to the first Brillouin zone and need to satisfy the constraint $\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4 = n\mathbf{G}$ with n an integer.

As the expressions of $\hat{b}_{k\uparrow,\downarrow}$ have even more terms, under the new representation, the expressions for interactions on the sublattices B will turn out to be too complicated. As the higher band almost has no effect on the ground state when the temperature is low, in fact we can neglect terms involving $\hat{\beta}_{1,2}$. Although in continuous system, it is found that the higher band can induce divergent effective interaction in the lower band [1], here the divergence behavior will be avoided since there is a natural cutoff, $2\pi/a$, for momentum, and if we consider the third dimension which is strongly confined, the infrared divergence is also absent. Therefore, in the following, for simplicity, we neglect all terms involving $\hat{\beta}_{1,2}$ and do not consider the renormalization of the interaction.

$$\begin{aligned}
& g_{1B} \sum_{k_1, k_2, k_3, k_4} \hat{b}_{k_1\uparrow}^\dagger \hat{b}_{k_2\uparrow}^\dagger \hat{b}_{k_3\uparrow} \hat{b}_{k_4\uparrow} \\
&= g_{1B} \sum_{k_1, k_2, k_3, k_4} (\lambda_4^*(k_1) \hat{\alpha}_{1k_1}^\dagger - \lambda_3^*(k_1) \hat{\alpha}_{2k_1}^\dagger) (\lambda_4^*(k_2) \hat{\alpha}_{1k_2}^\dagger - \lambda_3^*(k_2) \hat{\alpha}_{2k_2}^\dagger) (\lambda_4(k_3) \hat{\alpha}_{1k_3} - \lambda_3^*(k_3) \hat{\alpha}_{2k_3}) (\lambda_4(k_4) \hat{\alpha}_{1k_4} - \lambda_3^*(k_4) \hat{\alpha}_{2k_4}) \\
&= g_{1B} \sum_{k_1, k_2, k_3, k_4} [\lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} - 2\lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_4(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_3^*(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} - 2\lambda_4^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} \\
&\quad + 4\lambda_4^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} - 2\lambda_4^*(k_1) \lambda_3^*(k_2) \lambda_3^*(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} - 2\lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_3^*(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_3^*(k_3) \lambda_3^*(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}],
\end{aligned}$$

$$\begin{aligned}
& g_{1B} \sum_{k_1, k_2, k_3, k_4} \hat{b}_{k_1\downarrow}^\dagger \hat{b}_{k_2\downarrow}^\dagger \hat{b}_{k_3\downarrow} \hat{b}_{k_4\downarrow} \\
&= g_{1B} \sum_{k_1, k_2, k_3, k_4} (\lambda_3^*(k_1) \hat{\alpha}_{1k_1}^\dagger + \lambda_4^*(k_1) \hat{\alpha}_{2k_1}^\dagger) (\lambda_3^*(k_2) \hat{\alpha}_{1k_2}^\dagger + \lambda_4^*(k_2) \hat{\alpha}_{2k_2}^\dagger) (\lambda_3(k_4) \hat{\alpha}_{1k_4} + \lambda_4(k_4) \hat{\alpha}_{2k_4}) (\lambda_3(k_3) \hat{\alpha}_{1k_3} + \lambda_4(k_3) \hat{\alpha}_{2k_3}) \\
&= g_{1B} \sum_{k_1, k_2, k_3, k_4} [\lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_3(k_3) \lambda_3(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + 2\lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} + 2\lambda_3^*(k_1) \lambda_4^*(k_2) \lambda_3(k_3) \lambda_3(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} \\
&\quad + 4\lambda_3^*(k_1) \lambda_4^*(k_2) \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} + 2\lambda_3^*(k_1) \lambda_4^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_3(k_3) \lambda_3(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + 2\lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} \\
&\quad + \lambda_4^*(k_1) \lambda_4^*(k_2) \lambda_4(k_3) \lambda_4(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}],
\end{aligned}$$

$$\begin{aligned}
& 2g_{12B} \sum_{k_1, k_2, k_3, k_4} \hat{b}_{k_1\uparrow}^\dagger \hat{b}_{k_2\downarrow}^\dagger \hat{b}_{k_3\downarrow} \hat{b}_{k_4\uparrow} \\
&= 2g_{12B} \sum_{k_1, k_2, k_3, k_4} (\lambda_4^*(k_1) \hat{\alpha}_{1k_1}^\dagger - \lambda_3(k_1) \hat{\alpha}_{2k_1}^\dagger) (\lambda_3^*(k_2) \hat{\alpha}_{1k_2}^\dagger + \lambda_4^*(k_2) \hat{\alpha}_{2k_2}^\dagger) (\lambda_3(k_3) \hat{\alpha}_{1k_3} + \lambda_4(k_3) \hat{\alpha}_{2k_3}) (\lambda_4(k_4) \hat{\alpha}_{1k_4} - \lambda_3^*(k_4) \hat{\alpha}_{2k_4}) \\
&= 2g_{12B} \sum_{k_1, k_2, k_3, k_4} [\lambda_4^*(k_1) \lambda_3^*(k_2) \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + \lambda_4^*(k_1) \lambda_3^*(k_2) (\lambda_4(k_3) \lambda_4(k_4) - \lambda_3(k_3) \lambda_3^*(k_4)) \\
&\quad \times \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{2k_4} - \lambda_4^*(k_1) \lambda_3^*(k_2) \lambda_4(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} + (\lambda_4^*(k_1) \lambda_4^*(k_2) - \lambda_3^*(k_1) \lambda_3(k_2)) \\
&\quad \times \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + (\lambda_4^*(k_1) \lambda_4^*(k_2) - \lambda_3^*(k_1) \lambda_3(k_2)) (\lambda_4(k_3) \lambda_4(k_4) - \lambda_3^*(k_3) \lambda_3(k_4)) \\
&\quad \times \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4} - (\lambda_4^*(k_1) \lambda_4^*(k_2) - \lambda_3^*(k_1) \lambda_3(k_2)) \lambda_3(k_3) \lambda_3^*(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4} \\
&\quad - \lambda_3(k_1) \lambda_4^*(k_2) \lambda_3(k_3) \lambda_4(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} - \lambda_3(k_1) \lambda_4^*(k_2) (\lambda_4(k_3) \lambda_4(k_4) - \lambda_3(k_3) \lambda_3^*(k_4)) \\
&\quad \times \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger + \lambda_3(k_1) \lambda_4^*(k_2) \lambda_4(k_3) \lambda_3^*(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}]. \tag{20}
\end{aligned}$$

Although the interaction forms are very complicated, we only need to consider several of them when we are going to determine the ground state. For example, when the bosons are condensed at \mathbf{k}_0 or \mathbf{k}_π , as $\lambda_3(\mathbf{k}_0) = \lambda_3(\mathbf{k}_\pi) = 0$, in fact only the following terms have contribution to the energy of ground state,

$$\begin{aligned}
& \sum_{k_1, k_2, k_3, k_4} \{ \lambda_1(k_1) \lambda_1(k_2) \lambda_1(k_3) \lambda_1(k_4) [g_{1A} (\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}) + 2g_{12A} \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4}] \\
& \quad + \lambda_4(k_1) \lambda_4(k_2) \lambda_4(k_3) \lambda_4(k_4) [g_{1B} (\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}) + 2g_{12B} \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4}] \} \tag{21}
\end{aligned}$$

Therefore, the calculation is in fact not very tedious.

B. Ground state energy for $\alpha > \alpha_c$.

When $\alpha > \alpha_c$, the bosons will be condensed at $\mathbf{Q}_{1,2,3,4}$. As $\lambda_4(\mathbf{Q}_{1,2,3,4}) = 0$, the terms that have contribution to the ground state energy are given as

$$\begin{aligned}
& \sum_{k_1, k_2, k_3, k_4} \{ \lambda_1(k_1) \lambda_1(k_2) \lambda_1(k_3) \lambda_1(k_4) [g_{1A} (\hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}) + 2g_{12A} \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4}] \\
& \quad + g_{1B} (\lambda_3^*(k_1) \lambda_3^*(k_2) \lambda_3(k_3) \lambda_3(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{1k_2}^\dagger \hat{\alpha}_{1k_3} \hat{\alpha}_{1k_4} + \lambda_3(k_1) \lambda_3(k_2) \lambda_3^*(k_3) \lambda_3^*(k_4) \hat{\alpha}_{2k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{2k_4}) \\
& \quad + 2g_{12B} (\lambda_3^*(k_1) \lambda_3(k_2) \lambda_3^*(k_3) \lambda_3(k_4) \hat{\alpha}_{1k_1}^\dagger \hat{\alpha}_{2k_2}^\dagger \hat{\alpha}_{2k_3} \hat{\alpha}_{1k_4}) \}. \tag{22}
\end{aligned}$$

Combining Eq.(13) and Eq.(22), it is direct to obtain $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle$ whose concrete form is given as

$$\begin{aligned}
\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle = & \langle \tilde{\Psi}_f | H_{int} | \tilde{\Psi}_f \rangle + \{ 2U_{1,A} \frac{N_1 - 1}{N_1} [N_{11}N_{12} \cos(2\phi_{1,2}) + N_{11}N_{13} \cos(2\phi_{1,3}) + N_{11}N_{14} \cos(2\phi_{1,4}) \\
& + N_{12}N_{13} \cos 2(\phi_{1,3} - \phi_{1,2}) + N_{12}N_{14} \cos 2(\phi_{1,4} - \phi_{1,2}) + N_{13}N_{14} \cos 2(\phi_{1,4} - \phi_{1,3}) \\
& + 4\sqrt{N_{11}N_{12}N_{13}N_{14}} [\cos(\phi_{1,4} + \phi_{1,3} - \phi_{1,2}) + \cos(\phi_{1,2} + \phi_{1,3} - \phi_{1,4}) + \cos(\phi_{1,2} + \phi_{1,4} - \phi_{1,3})] \} \\
& + 2U_{1,A} \frac{N_2 - 1}{N_2} [N_{21}N_{22} \cos(2\phi_{2,2}) + N_{21}N_{23} \cos(2\phi_{2,3}) + N_{21}N_{24} \cos(2\phi_{2,4}) + N_{22}N_{23} \cos 2(\phi_{2,3} - \phi_{2,2}) \\
& + N_{22}N_{24} \cos 2(\phi_{2,4} - \phi_{2,2}) + N_{23}N_{24} \cos 2(\phi_{2,4} - \phi_{2,3}) + 4\sqrt{N_{21}N_{22}N_{23}N_{24}} [\cos(\phi_{2,4} + \phi_{2,3} - \phi_{2,2}) \\
& + \cos(\phi_{2,2} + \phi_{2,3} - \phi_{2,4}) + \cos(\phi_{2,2} + \phi_{2,4} - \phi_{2,3})] + 8U_{2,A} [\sqrt{N_{11}N_{12}N_{21}N_{22}} \cos(\phi_{1,2}) \cos(\phi_{2,2}) \\
& + \sqrt{N_{11}N_{13}N_{21}N_{23}} \cos(\phi_{1,3}) \cos(\phi_{2,3}) + \sqrt{N_{11}N_{14}N_{21}N_{24}} \cos(\phi_{1,4}) \cos(\phi_{2,4}) + \sqrt{N_{12}N_{13}N_{22}N_{23}} \\
& * \cos(\phi_{1,3} - \phi_{1,2}) \cos(\phi_{2,3} - \phi_{2,2}) + \sqrt{N_{12}N_{14}N_{22}N_{24}} \cos(\phi_{1,4} - \phi_{1,2}) \cos(\phi_{2,4} - \phi_{2,2}) \\
& + \sqrt{N_{13}N_{14}N_{22}N_{23}} \cos(\phi_{1,4} - \phi_{1,3}) \cos(\phi_{2,4} - \phi_{2,3})] + 8U_{2,A} [\sqrt{N_{11}N_{12}N_{23}N_{24}} \cos(\phi_{1,2}) \cos(\phi_{2,4} - \phi_{2,3}) \\
& + \sqrt{N_{11}N_{13}N_{22}N_{24}} \cos(\phi_{1,3}) \cos(\phi_{2,4} - \phi_{2,2}) + \sqrt{N_{11}N_{14}N_{22}N_{23}} \cos(\phi_{1,4}) \cos(\phi_{2,3} - \phi_{2,2}) \\
& + \sqrt{N_{12}N_{13}N_{21}N_{24}} \cos(\phi_{1,3} - \phi_{1,2}) \cos(\phi_{2,4}) + \sqrt{N_{12}N_{14}N_{21}N_{23}} \cos(\phi_{1,4} - \phi_{1,2}) \cos(\phi_{2,3}) \\
& + \sqrt{N_{13}N_{14}N_{21}N_{22}} \cos(\phi_{1,4} - \phi_{1,3}) \cos(\phi_{2,2})] \} \cos^4(\tilde{\theta}/2) + \{ 2U_{1,B} \frac{N_1 - 1}{N_1} [N_{11}N_{12} \cos(2\phi_{1,2}) \\
& - N_{11}N_{13} \cos(2\phi_{1,3}) - N_{11}N_{14} \cos(2\phi_{1,4}) - N_{12}N_{13} \cos 2(\phi_{1,3} - \phi_{1,2}) - N_{12}N_{14} \cos 2(\phi_{1,4} - \phi_{1,2}) \\
& + N_{13}N_{14} \cos 2(\phi_{1,4} - \phi_{1,3}) + 4\sqrt{N_{11}N_{12}N_{13}N_{14}} [-\cos(\phi_{1,4} + \phi_{1,3} - \phi_{1,2}) + \cos(\phi_{1,2} + \phi_{1,3} - \phi_{1,4}) \\
& + \cos(\phi_{1,2} + \phi_{1,4} - \phi_{1,3})] + 2U_{1,B} \frac{N_2 - 1}{N_2} [N_{21}N_{22} \cos(2\phi_{2,2}) - N_{21}N_{23} \cos(2\phi_{2,3}) - N_{21}N_{24} \cos(2\phi_{2,4}) \\
& - N_{22}N_{23} \cos 2(\phi_{2,3} - \phi_{2,2}) - N_{22}N_{24} \cos 2(\phi_{2,4} - \phi_{2,2}) + N_{23}N_{24} \cos 2(\phi_{2,4} - \phi_{2,3}) \\
& + 4\sqrt{N_{21}N_{22}N_{23}N_{24}} [-\cos(\phi_{2,4} + \phi_{2,3} - \phi_{2,2}) + \cos(\phi_{2,2} + \phi_{2,3} - \phi_{2,4}) + \cos(\phi_{2,2} + \phi_{2,4} - \phi_{2,3})] \} \\
& + 8U_{2,B} [\sqrt{N_{11}N_{12}N_{21}N_{22}} \cos(\phi_{1,2}) \cos(\phi_{2,2}) - \sqrt{N_{11}N_{13}N_{21}N_{23}} \sin(\phi_{1,3}) \sin(\phi_{2,3}) \\
& - \sqrt{N_{11}N_{14}N_{21}N_{24}} \sin(\phi_{1,4}) \sin(\phi_{2,4}) - \sqrt{N_{12}N_{13}N_{22}N_{23}} \sin(\phi_{1,3} - \phi_{1,2}) \sin(\phi_{2,3} - \phi_{2,2}) \\
& - \sqrt{N_{12}N_{14}N_{22}N_{24}} \sin(\phi_{1,4} - \phi_{1,2}) \sin(\phi_{2,4} - \phi_{2,2}) + \sqrt{N_{13}N_{14}N_{22}N_{23}} \cos(\phi_{1,4} - \phi_{1,3}) \cos(\phi_{2,4} - \phi_{2,3})] \\
& + 8U_{2,B} [\sqrt{N_{11}N_{12}N_{23}N_{24}} \cos(\phi_{1,2}) \cos(\phi_{2,4} - \phi_{2,3}) + \sqrt{N_{11}N_{13}N_{22}N_{24}} \sin(\phi_{1,3}) \sin(\phi_{2,4} - \phi_{2,2}) \\
& + \sqrt{N_{11}N_{14}N_{22}N_{23}} \sin(\phi_{1,4}) \sin(\phi_{2,3} - \phi_{2,2}) + \sqrt{N_{12}N_{13}N_{21}N_{24}} \sin(\phi_{1,3} - \phi_{1,2}) \sin(\phi_{2,4}) \\
& + \sqrt{N_{12}N_{14}N_{21}N_{23}} \sin(\phi_{1,4} - \phi_{1,2}) \sin(\phi_{2,3}) + \sqrt{N_{13}N_{14}N_{21}N_{22}} \cos(\phi_{1,4} - \phi_{1,3}) \cos(\phi_{2,2})] \} \sin^4(\tilde{\theta}/2).
\end{aligned}$$

When the bosons are condensed at only one of the minima, for example, at \mathbf{Q}_1 , then $N_{11} = N_1$ and $N_{21} = N_2$, $N_{1i} = N_{2i} = 0$ with $i \neq 1$. As a result, it is easy to see that $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle = \langle \tilde{\Psi}_f | H_{int} | \tilde{\Psi}_f \rangle = \tilde{E}_s$. When the bosons are only simultaneously condensed at two minima which are time-reversal partner, for example, \mathbf{Q}_1 and \mathbf{Q}_2 , then the above equation is greatly simplified,

$$\begin{aligned}
\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle = & \langle \tilde{\Psi}_f | H_{int} | \tilde{\Psi}_f \rangle + \{ 2U_{1,A} \frac{N_1 - 1}{N_1} [N_{11}N_{12} \cos(2\phi_{1,2})] + 2U_{1,B} \frac{N_1 - 1}{N_1} [N_{11}N_{12} \cos(2\phi_{1,2})] \\
& + [(N_1, N_{1i}, \phi_{1,i}) \longleftrightarrow (N_2, N_{2i}, \phi_{2,i})] \} + 8U_{2,A} [\sqrt{N_{11}N_{12}N_{21}N_{22}} \cos(\phi_{1,2}) \cos(\phi_{2,2})] \\
& + 8U_{2,B} [\sqrt{N_{11}N_{12}N_{21}N_{22}} \cos(\phi_{1,2}) \cos(\phi_{2,2})].
\end{aligned} \tag{23}$$

When $U_1 > U_2$, by minimizing the energy, it is found that $N_{11}, N_{12}, N_{21}, N_{22}$ can takes arbitrary values if $\phi_{1,2}, \phi_{2,2}$ are locked to $\{(n + \frac{1}{2})\pi, n \in Z\}$, and the minimum value of $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle$ is also \tilde{E}_s . However, if the bosons are simultaneously condensed at two minima that are not time-reversal partner, for example, \mathbf{Q}_1 and \mathbf{Q}_3 , it is found that the minimum value of $\langle \tilde{\Psi}_c | H_{int} | \tilde{\Psi}_c \rangle$ is given as $\tilde{E}_s + 4[U_{1,B}(N_{11}N_{13} + N_{21}N_{23}) - 2U_{2,B}\sqrt{N_{11}N_{13}N_{21}N_{23}}] \sin^4(\tilde{\theta}/2)$, which is larger than \tilde{E}_s , and therefore, it is not favored in energy. Other cases can be similarly discussed and we neglect the discussion here.

C. Particle distribution for $\alpha > \alpha_c$.

$$\begin{aligned}
|\varphi_{A\uparrow}(\mathbf{r}_i)|^2 &= n_0 \tilde{\chi}_1^2 (1 + 2|b_1||b_3| \cos(\frac{\pi(x_i + y_i)}{a} - \varphi_{13}) + 2|b_1||b_5| \cos(\frac{\pi y_i}{a} - \varphi_{15}) + 2|b_1||b_7| \cos(\frac{\pi x_i}{a} - \varphi_{17}) \\
&\quad + 2|b_3||b_5| \cos(\frac{\pi x_i}{a} + \varphi_{35}) + 2|b_3||b_7| \cos(\frac{\pi y_i}{a} + \varphi_{37}) + 2|b_5||b_7| \cos(\frac{\pi(x_i - y_i)}{a} - \varphi_{57})) \xi_1. \\
|\varphi_{B\downarrow}(\mathbf{r}_i)|^2 &= n_0 \tilde{\chi}_2^2 (1 - 2|b_1||b_3| \cos(\frac{\pi(x_i + y_i)}{a} - \varphi_{13}) - 2|b_1||b_5| \sin(\frac{\pi y_i}{a} - \varphi_{15}) + 2|b_1||b_7| \sin(\frac{\pi x_i}{a} - \varphi_{17}) \\
&\quad - 2|b_3||b_5| \sin(\frac{\pi x_i}{a} + \varphi_{35}) + 2|b_3||b_7| \sin(\frac{\pi y_i}{a} + \varphi_{37}) - 2|b_5||b_7| \cos(\frac{\pi(x_i - y_i)}{a} - \varphi_{57})) \xi_2. \\
|\varphi_{B\uparrow}(\mathbf{r}_i)|^2 &= n_0 \tilde{\chi}_1^2 (1 - 2|b_2||b_4| \cos(\frac{\pi(x_i + y_i)}{a} - \varphi_{24}) + 2|b_2||b_6| \sin(\frac{\pi y_i}{a} - \varphi_{26}) - 2|b_2||b_8| \sin(\frac{\pi x_i}{a} - \varphi_{28}) \\
&\quad + 2|b_4||b_6| \sin(\frac{\pi x_i}{a} + \varphi_{46}) - 2|b_4||b_8| \sin(\frac{\pi y_i}{a} + \varphi_{48}) - 2|b_6||b_8| \cos(\frac{\pi(x_i - y_i)}{a} - \varphi_{68})) \xi_2. \\
|\varphi_{A\downarrow}(\mathbf{r}_i)|^2 &= n_0 \tilde{\chi}_1^2 (1 + 2|b_2||b_4| \cos(\frac{\pi(x_i + y_i)}{a} - \varphi_{24}) + 2|b_2||b_6| \cos(\frac{\pi y_i}{a} - \varphi_{26}) + 2|b_2||b_8| \cos(\frac{\pi x_i}{a} - \varphi_{28}) \\
&\quad + 2|b_4||b_6| \cos(\frac{\pi x_i}{a} + \varphi_{46}) + 2|b_2||b_4| \cos(\frac{\pi y_i}{a} + \varphi_{48}) + 2|b_6||b_8| \cos(\frac{\pi(x_i - y_i)}{a} - \varphi_{68})) \xi_1.
\end{aligned} \tag{24}$$

$|b_{i \in odd}|$ correspond to $\hat{\alpha}_1$, while $|b_{i \in even}|$ correspond to $\hat{\alpha}_2$.

When only one of $|b_{i \in odd}|$ and one of $|b_{i \in even}|$ are nonzero, it is direct to see that $|\varphi_{A\uparrow}(\mathbf{r}_i)|^2 = |\varphi_{A\downarrow}(\mathbf{r}_i)|^2 = n_0 \tilde{\chi}_1^2$, $|\varphi_{B\uparrow}(\mathbf{r}_i)|^2 = |\varphi_{B\downarrow}(\mathbf{r}_i)|^2 = n_0 \tilde{\chi}_2^2$, which corresponds to a spin-balanced condensate. When the bosons are condensed at two minima which are time-reversal partner, for example, \mathbf{Q}_1 and \mathbf{Q}_2 , then only $b_{1,2,3,4}$ are nonzero. When φ_{13} (equivalent to $\phi_{1,2}$) and φ_{24} (equivalent to $\phi_{2,2}$) are locked to $\{(n + \frac{1}{2})\pi, n \in \mathbb{Z}\}$, it is easy to see that the spin configuration is the same as the former single minimum occupied case, with $|\varphi_{A\uparrow}(\mathbf{r}_i)|^2 = |\varphi_{A\downarrow}(\mathbf{r}_i)|^2 = n_0 \tilde{\chi}_1^2$, $|\varphi_{B\uparrow}(\mathbf{r}_i)|^2 = |\varphi_{B\downarrow}(\mathbf{r}_i)|^2 = n_0 \tilde{\chi}_2^2$. A discussion of the spin configuration corresponding to other possible ground states is similar and we neglect it here.

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[1] T. Ozawa and G. Baym, Phys. Rev. A **84**, 043622 (2011).